LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071723\
Data File : BF134329.D
Acq On : 17 Jul 2023 22:38
Operator : CG\JU
Sample : 03597-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RB-42-(1-3)

Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF134329.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.075	505	508	518	rVB	18281	24226	1.68%	0.191%
2	5.475	571	576	590	rBV	1353479	1393103	96.82%	11.011%
3	6.481	742	747	765	rBV	1359929	1438829	100.00%	11.373%
4	6.669	776	779	790	rBV	30879	41877	2.91%	0.331%
5	6.840	804	808	817	rBV	460187	415601	28.88%	3.285%
6	7.398	899	903	913	rBV	1026775	872131	60.61%	6.893%
7	8.116	1021	1025	1028	rBV	669567	509476	35.41%	4.027%
8	9.192	1204	1208	1211	rBV	1778808	1321333	91.83%	10.444%
9	9.304	1224	1227	1232	rVB	24479	22473	1.56%	0.178%
10	9.875	1320	1324	1327	rBV	628470	502552	34.93%	3.972%
11	10.633	1449	1453	1455	rBV2	18621	21476	1.49%	0.170%
12	10.669	1455	1459	1468	rVB	1059140	921521	64.05%	7.284%
13	10.798	1477	1481	1486	rVB	78498	77324	5.37%	0.611%
14	10.845	1486	1489	1492	rBV	187227	186625	12.97%	1.475%
15	10.880	1492	1495	1498	rVV2	202568	249176	17.32%	1.970%
16	10.916	1498	1501	1503	rVV	211990	200579	13.94%	1.585%
17	10.939	1503	1505	1508	rVV	121766	105539	7.34%	0.834%
18	10.980	1508	1512	1513	rVV2	61579	87797	6.10%	0.694%
19	10.998	1513	1515	1517	rVV	62347	58375	4.06%	0.461%
20	11.028	1517	1520	1524	rVV3	141782	175761	12.22%	1.389%
21	11.063	1524	1526	1529	rVV	190212	184667	12.83%	1.460%
22	11.104	1531	1533	1539	rVB	99426	96795	6.73%	0.765%
23	11.257	1555	1559	1564	rVB4	15097	24530	1.70%	0.194%
24	11.369	1574	1578	1580	rBV	601376	480257	33.38%	3.796%
25	11.392	1580	1582	1585	rVV	110918	94649	6.58%	0.748%
26	11.445	1588	1591	1594	rVB	23738	23340	1.62%	0.184%
27	11.869	1659	1663	1665	rBV2	29927	34671	2.41%	0.274%
28	11.898	1665	1668	1671	rVV2	194285	190099	13.21%	1.503%
29	11.927	1671	1673	1679	rVV	83420	95019	6.60%	0.751%
30	11.986	1679	1683	1685	rVV2	40100	47318	3.29%	0.374%
31	12.010	1685	1687	1691	rVB	19066	17311	1.20%	0.137%
32	12.204	1717	1720	1725	rVB4	15112	17642	1.23%	0.139%
33	12.427	1754	1758	1760	rBV	22876	26273	1.83%	0.208%
34	12.463	1760	1764	1770	rVB7	17950	36855	2.56%	0.291%
35	12.516	1770	1773	1777	rBV4	18694	22254	1.55%	0.176%
36	12.592	1782	1786	1789	rBV	213518	207984	14.46%	1.644%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071723\
Data File : BF134329.D
Acq On : 17 Jul 2023 22:38
Operator : CG\JU
Sample : 03597-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RB-42-(1-3)

Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	12.686	1800	1802	1807	rBV4	32638	41352	2.87%	0.327%
38	12.822	1820	1825	1829	rBV	217007	226128	15.72%	1.787%
39	12.963	1845	1849	1853	rBV	1227890	1060170	73.68%	8.380%
40	13.039	1859	1862	1869	rVB5	18990	26517	1.84%	0.210%
41	13.133	1874	1878	1879	rVV4	19706	26204	1.82%	0.207%
42	13.151	1879	1881	1884	rVB2	39622	35296	2.45%	0.279%
43	13.222	1890	1893	1895	rVB	22835	18871	1.31%	0.149%
44	13.257	1896	1899	1903	rVB2	26812	24916	1.73%	0.197%
45	13.380	1918	1920	1924	rBV2	19665	19301	1.34%	0.153%
46	13.886	2003	2006	2013	rVB6	53928	92212	6.41%	0.729%
47	14.027	2026	2030	2033	rBV2	346093	376176	26.14%	2.973%
48	14.057	2033	2035	2040	rVB	81790	75832	5.27%	0.599%
49	15.092	2208	2211	2214	rBV2	56507	81295	5.65%	0.643%
50	15.474	2273	2276	2281	rVB	49383	62096	4.32%	0.491%
51	15.533	2282	2286	2295	rVV	183193	259904	18.06%	2.054%

Sum of corrected areas: 12651708

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ClientSampleId :
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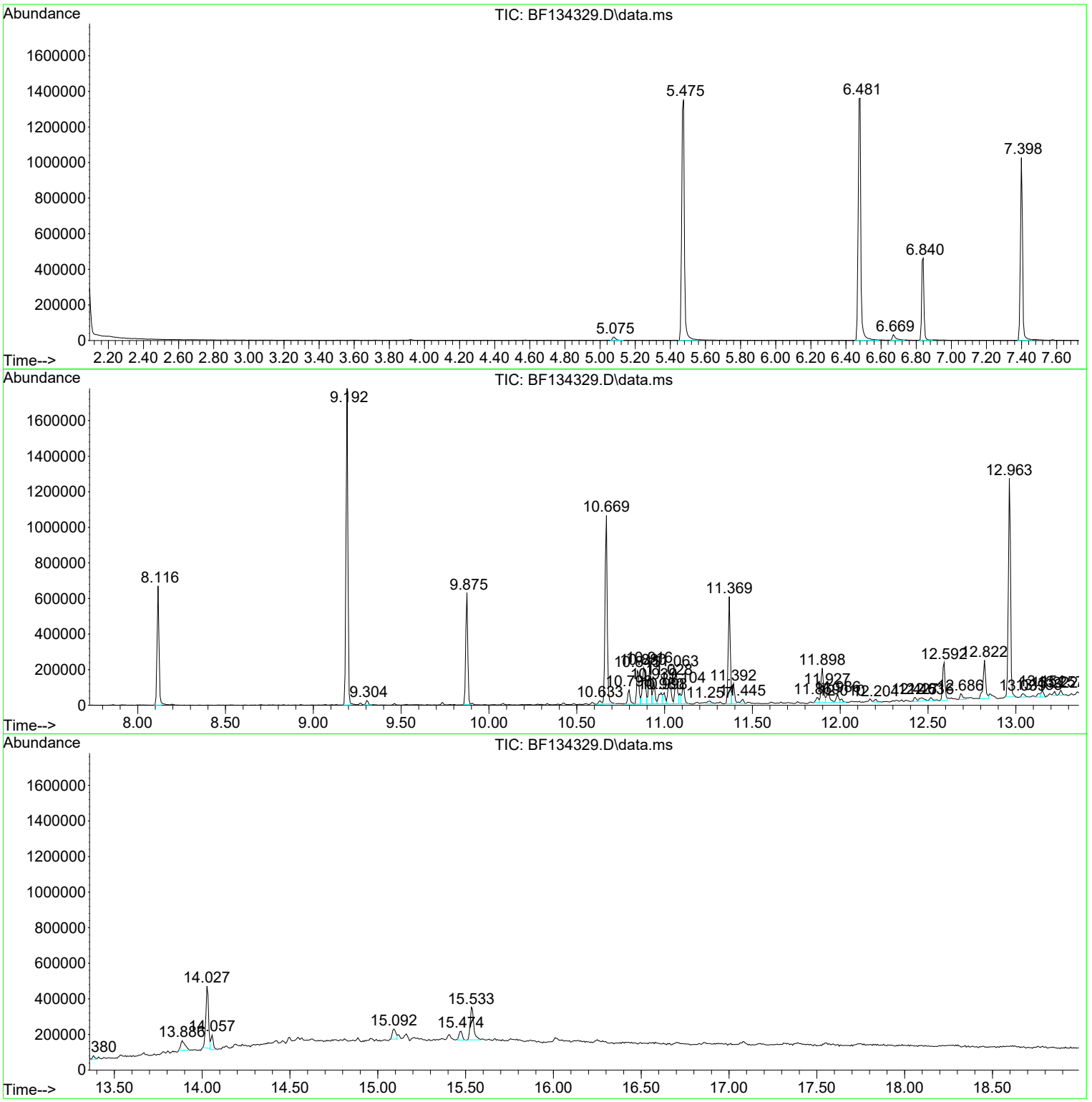
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071723\
Data File : BF134329.D
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Operator : CG\JU
Sample : 03597-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RB-42-(1-3)

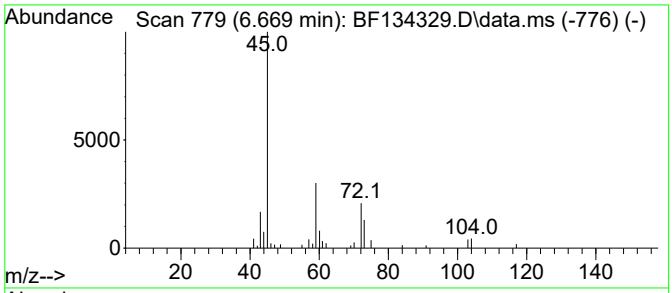
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

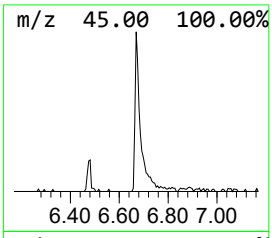
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

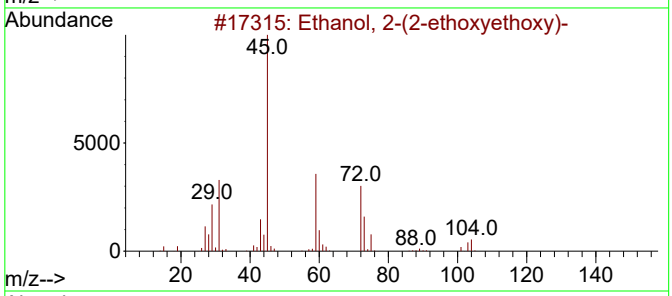
****
Peak Number 1 Ethanol, 2-(2-ethoxyethoxy)- Concentration Rank 12

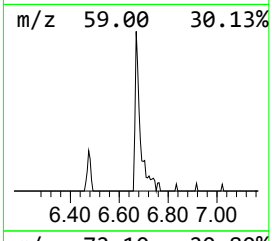
R.T.	EstConc	Area	Relative to ISTD	R.T.
6.669	2.02 ng	41877	1,4-Dichlorobenzene-d4	6.840

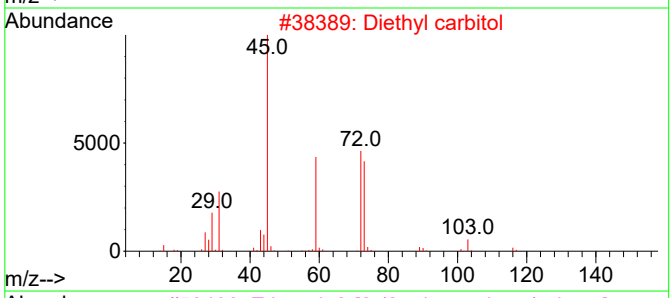
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-ethoxyethoxy)-	134	C6H14O3	000111-90-0	78
2	Diethyl carbitol	162	C8H18O3	000112-36-7	72
3	Ethanol, 2-[2-(2-ethoxyethoxy)et...	178	C8H18O4	000112-50-5	56
4	Methoxymethyl isothiocyanate	103	C3H5NOS	019900-84-6	53
5	Ethanol, 2-(2-methoxyethoxy)-	120	C5H12O3	000111-77-3	42

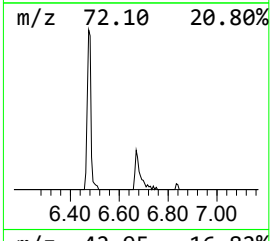


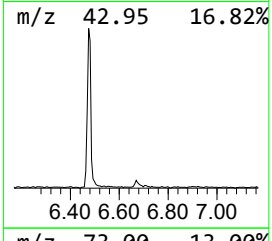


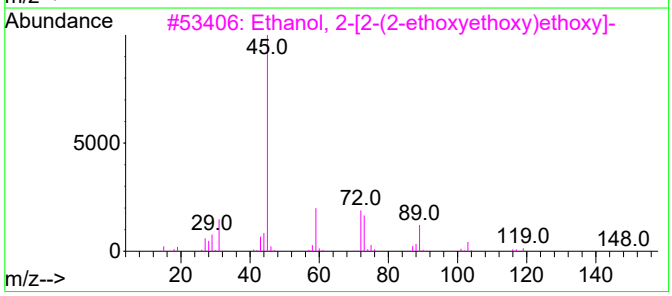


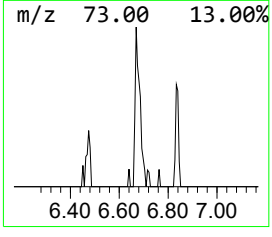












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Instrument :
BNA_F
ClientSampleId :
RB-42-(1-3)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

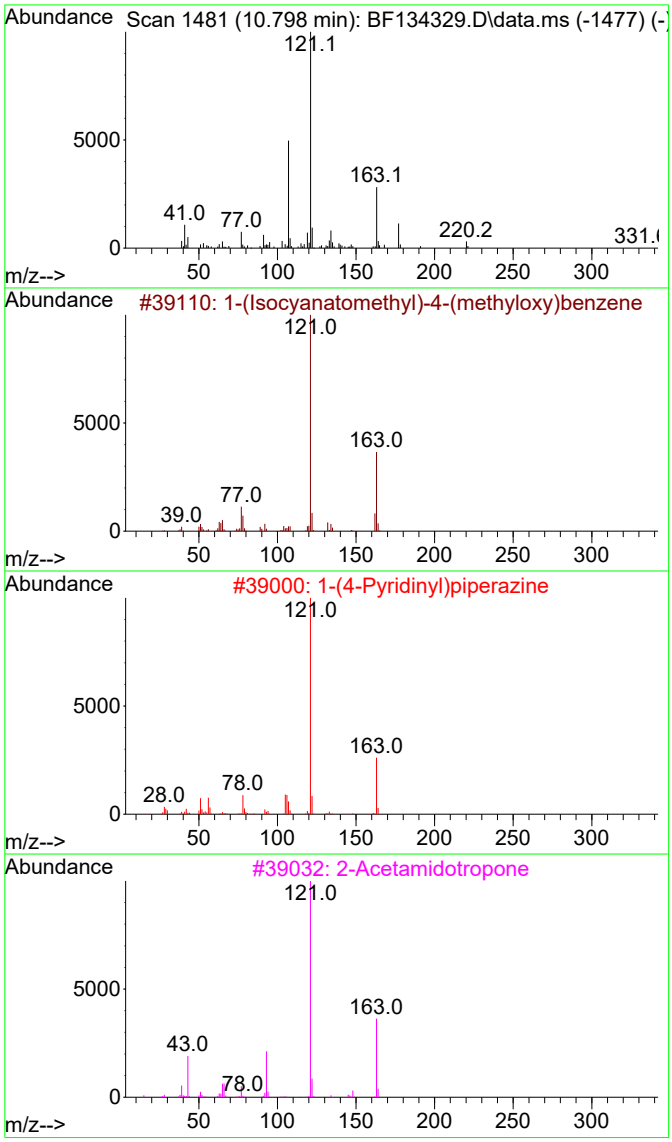
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

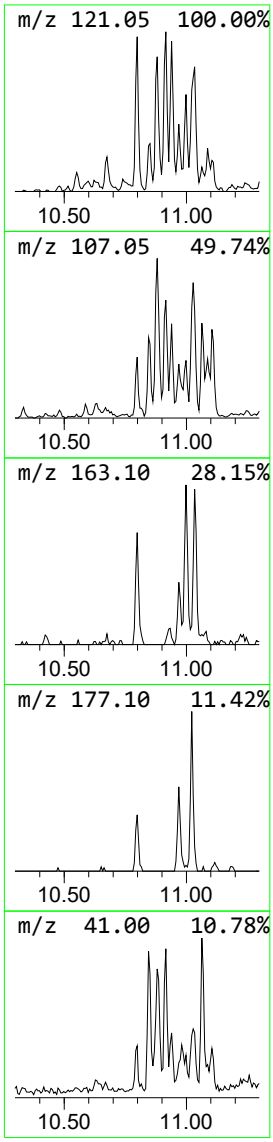
****

Peak Number 2 1-(Isocyanatomethyl)-4-(met... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.798	3.22 ng	77324	Phenanthrene-d10	11.369

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-(Isocyanatomethyl)-4-(methylox...	163	C9H9NO2	056651-60-6	50
2	1-(4-Pyridinyl)piperazine	163	C9H13N3	001008-91-9	50
3	2-Acetamidotropone	163	C9H9NO2	006422-12-4	47
4	N-Allyl-p-hydroxybenzamide	177	C10H11NO2	090921-72-5	43
5	4-sec-Butylphenol, O-(n-propylox...	236	C14H20O3	1000487-26-7	43





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BNA_F
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RB-42-(1-3)

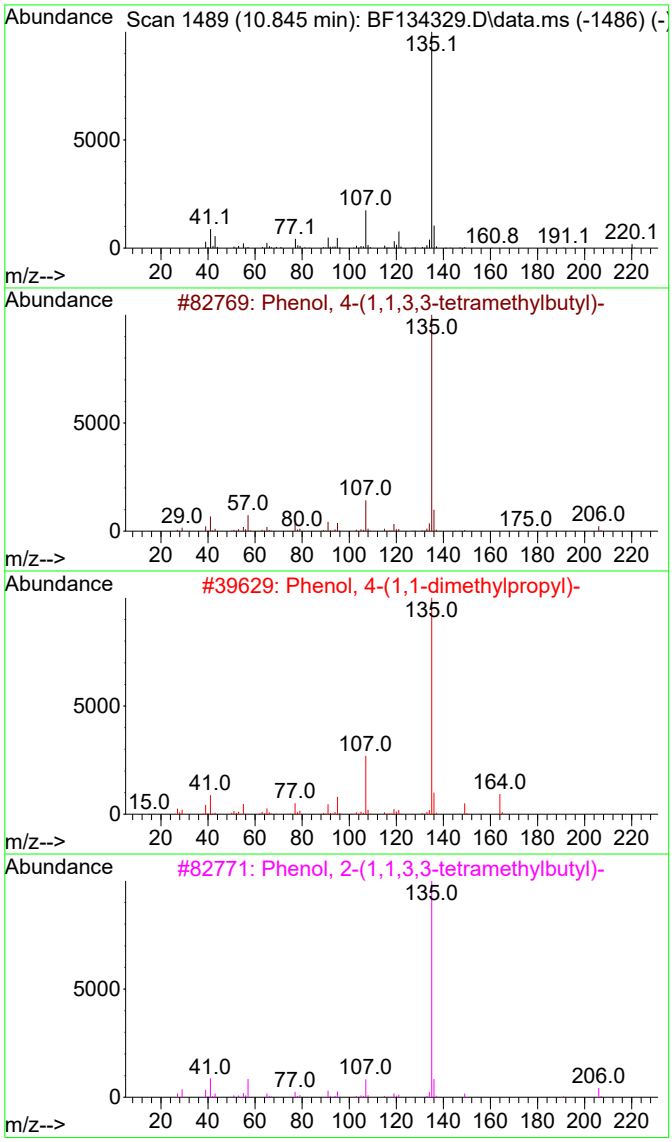
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

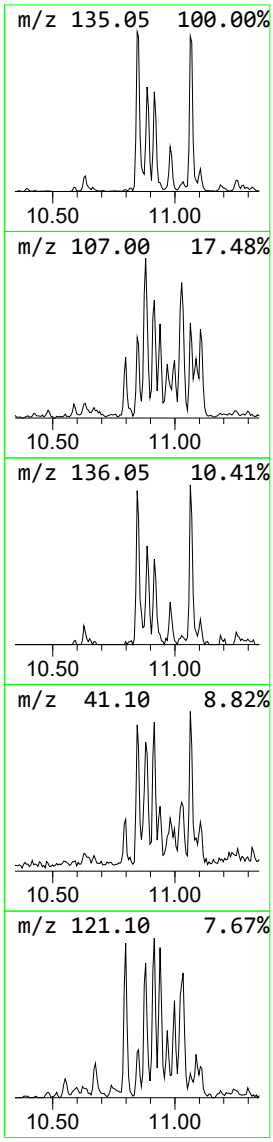
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Phenol, 4-(1,1,3,3-tetramet... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.845	7.77 ng	186625	Phenanthrene-d10	11.369

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 4-(1,1,3,3-tetramethylbu...	206	C14H22O	000140-66-9	86
2	Phenol, 4-(1,1-dimethylpropyl)-	164	C11H16O	000080-46-6	78
3	Phenol, 2-(1,1,3,3-tetramethylbu...	206	C14H22O	003884-95-5	78
4	4-(1,1-Dimethylpropyl)phenyl ace...	206	C13H18O2	1000373-45-3	78
5	4-tert-Butylphenyl acetate	192	C12H16O2	003056-64-2	78





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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

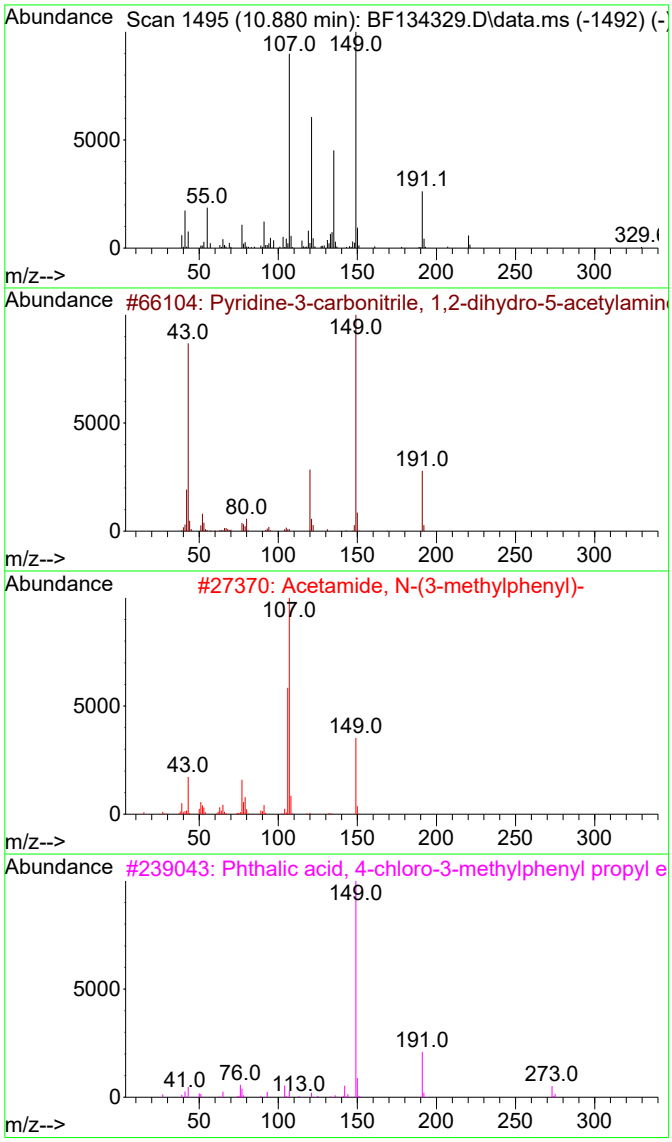
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

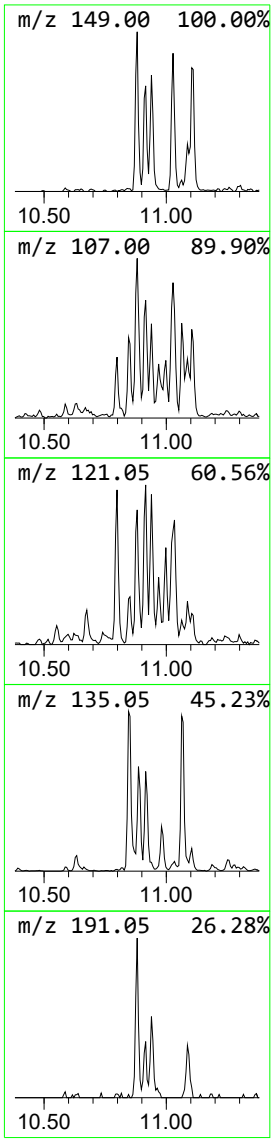
****

Peak Number 4 unknown10.881 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.881	10.38 ng	249176	Phenanthrene-d10	11.369

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pyridine-3-carbonitrile, 1,2-dih...	191	C9H9N3O2	220098-92-0	38
2	Acetamide, N-(3-methylphenyl)-	149	C9H11NO	000537-92-8	38
3	Phthalic acid, 4-chloro-3-methyl...	332	C18H17ClO4	1000309-84-2	35
4	Phthalic acid, 2-methylphenyl pr...	298	C18H18O4	1000314-95-1	35
5	Phenylpropionic acid pentafluoro...	330	C16H11F5O2	062434-95-1	27





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ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RB-42-(1-3)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

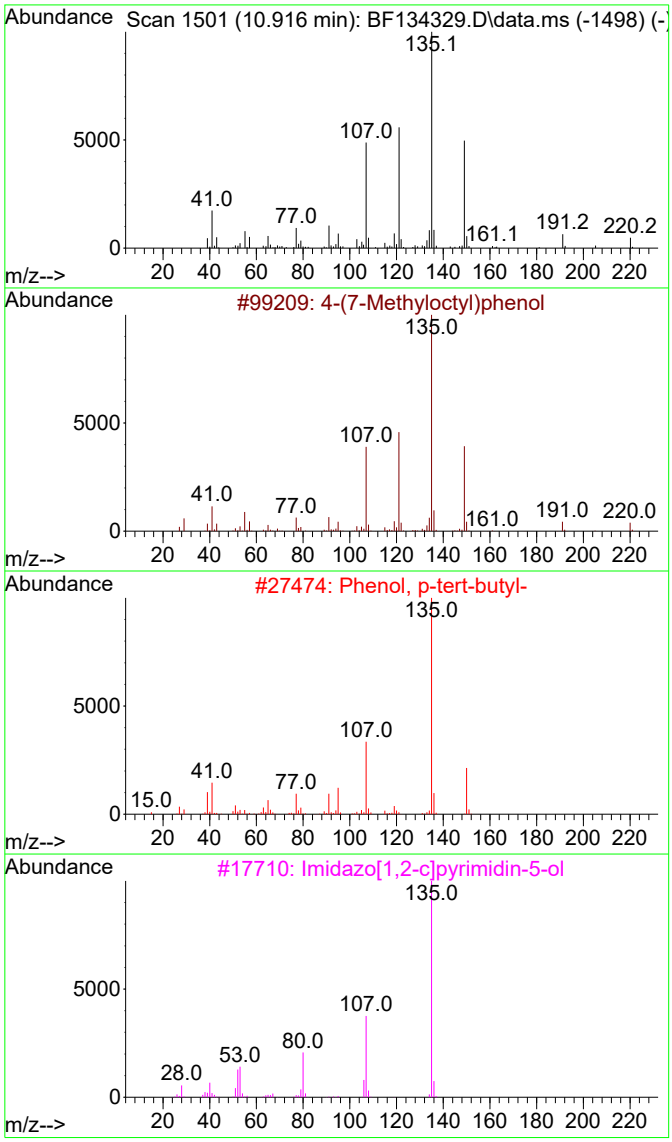
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

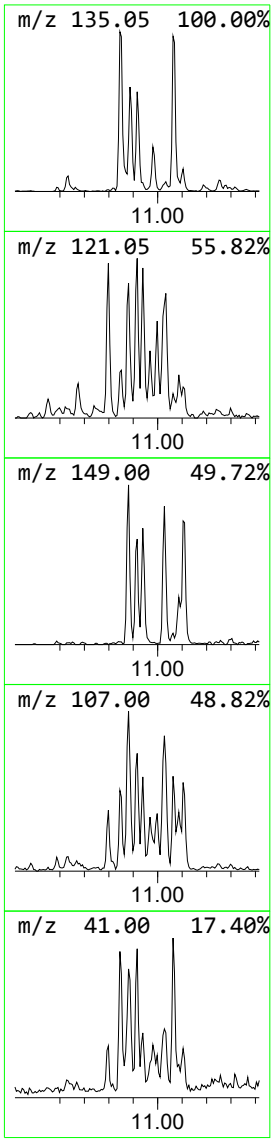
****

Peak Number 5 4-(7-Methyloctyl)phenol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.916	8.35 ng	200579	Phenanthrene-d10	11.369

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-(7-Methyloctyl)phenol	220	C15H24O	024518-48-7	98
2	Phenol, p-tert-butyl-	150	C10H14O	000098-54-4	58
3	Imidazo[1,2-c]pyrimidin-5-ol	135	C6H5N3O	055662-66-3	52
4	4-(1,1-Dimethylheptyl)phenol	220	C15H24O	1000384-80-3	50
5	1,5,6,7-Tetrahydro-4-indolone	135	C8H9NO	013754-86-4	50





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Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

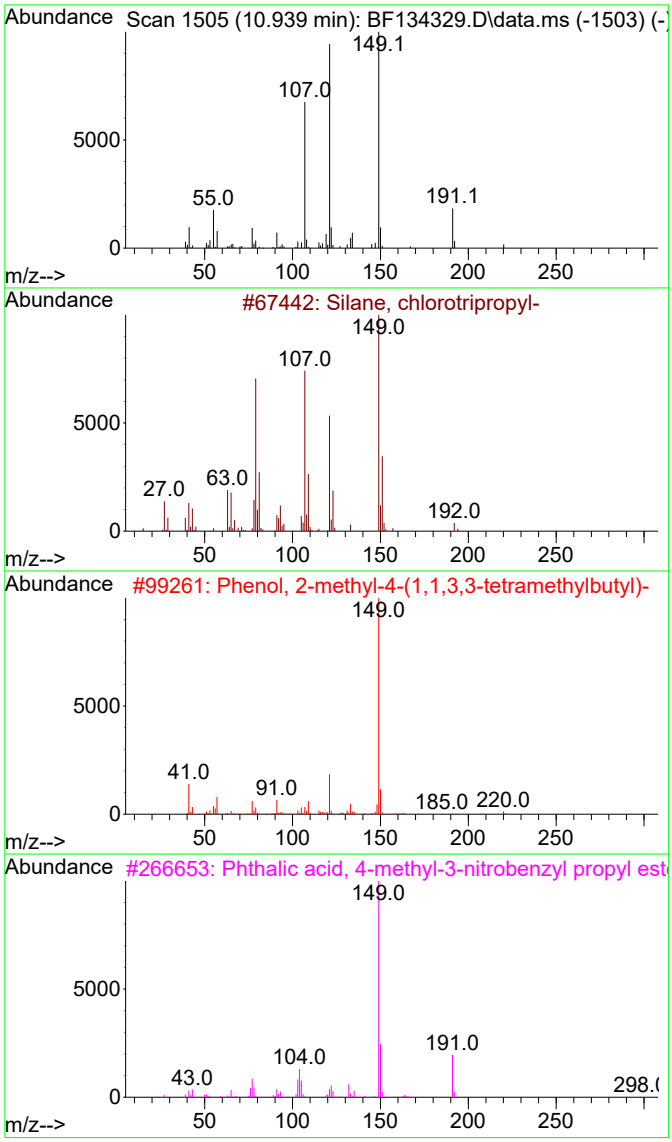
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

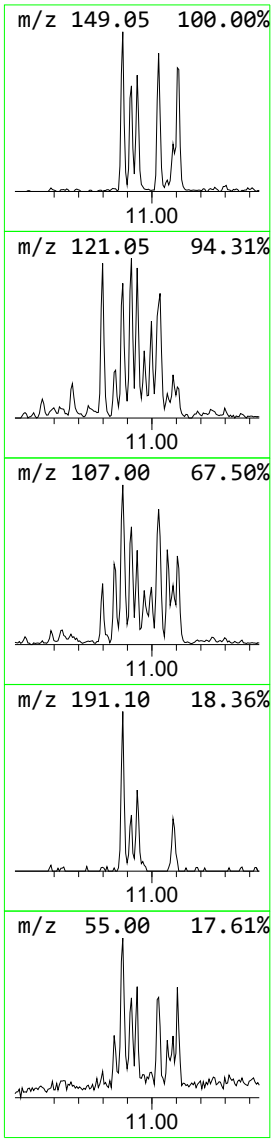
****

Peak Number 6 unknown10.939 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.939	4.40 ng	105539	Phenanthrene-d10	11.369

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Silane, chlorotripropyl-	192	C9H21ClSi	000995-25-5	47
2	Phenol, 2-methyl-4-(1,1,3,3-tetr...	220	C15H24O	002219-84-3	38
3	Phthalic acid, 4-methyl-3-nitrob...	357	C19H19NO6	1010382-58-0	35
4	4-Hydroxyphenylpyruvic acid, met...	208	C11H12O4	1000332-83-9	35
5	Isoxazole, 4,5-dihydro-5-[(4-met...	191	C11H13NO2	1010362-14-0	30





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Misc :
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Instrument :
BNA_F
ClientSampleId :
RB-42-(1-3)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

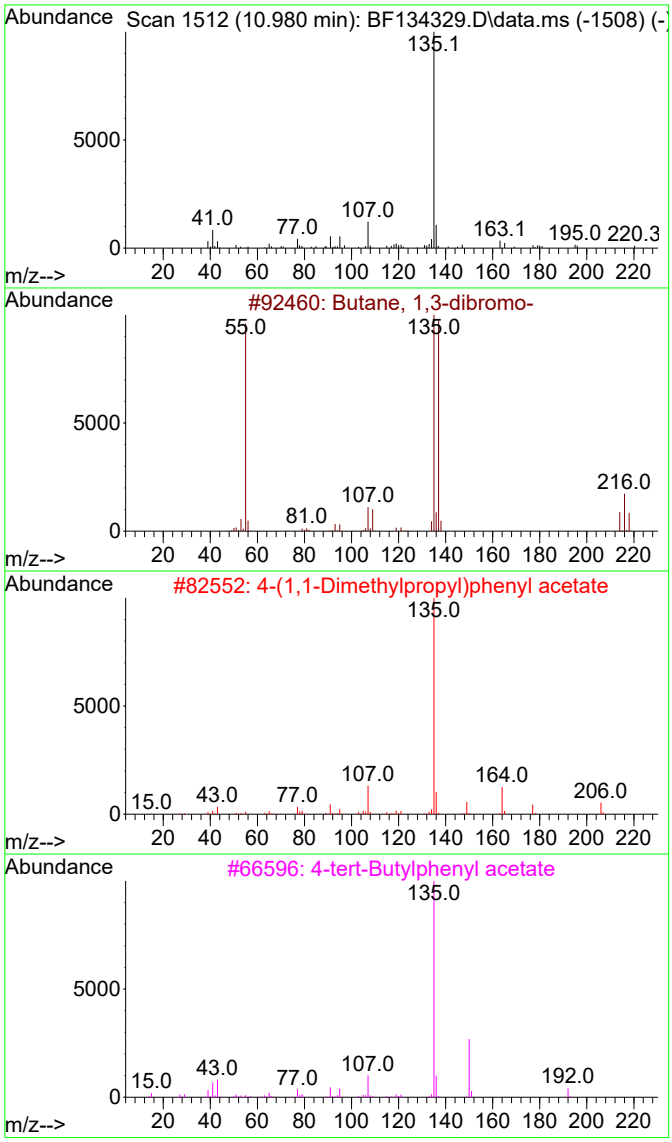
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

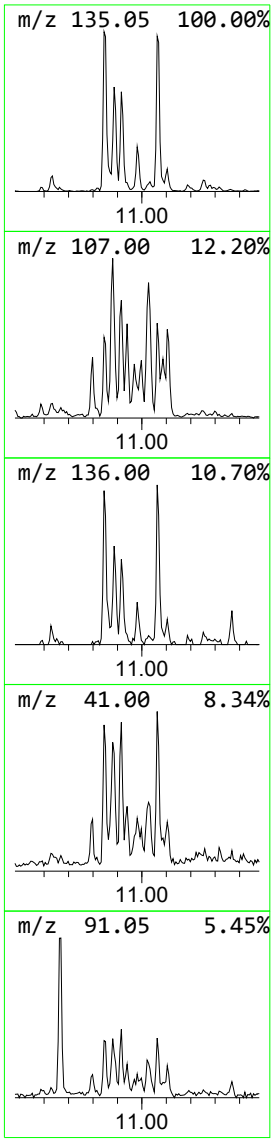
****

Peak Number 7 Butane, 1,3-dibromo- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.980	3.66 ng	87797	Phenanthrene-d10	11.369

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 1,3-dibromo-	214	C4H8Br2	000107-80-2	72
2	4-(1,1-Dimethylpropyl)phenyl ace...	206	C13H18O2	1000373-45-3	72
3	4-tert-Butylphenyl acetate	192	C12H16O2	003056-64-2	72
4	Phenol, 4-(1,1,3,3-tetramethylbu...	206	C14H22O	000140-66-9	72
5	Phenol, 2-(1,1,3,3-tetramethylbu...	206	C14H22O	003884-95-5	72





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Acq On : 17 Jul 2023 22:38
Operator : CG\JU
Sample : 03597-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RB-42-(1-3)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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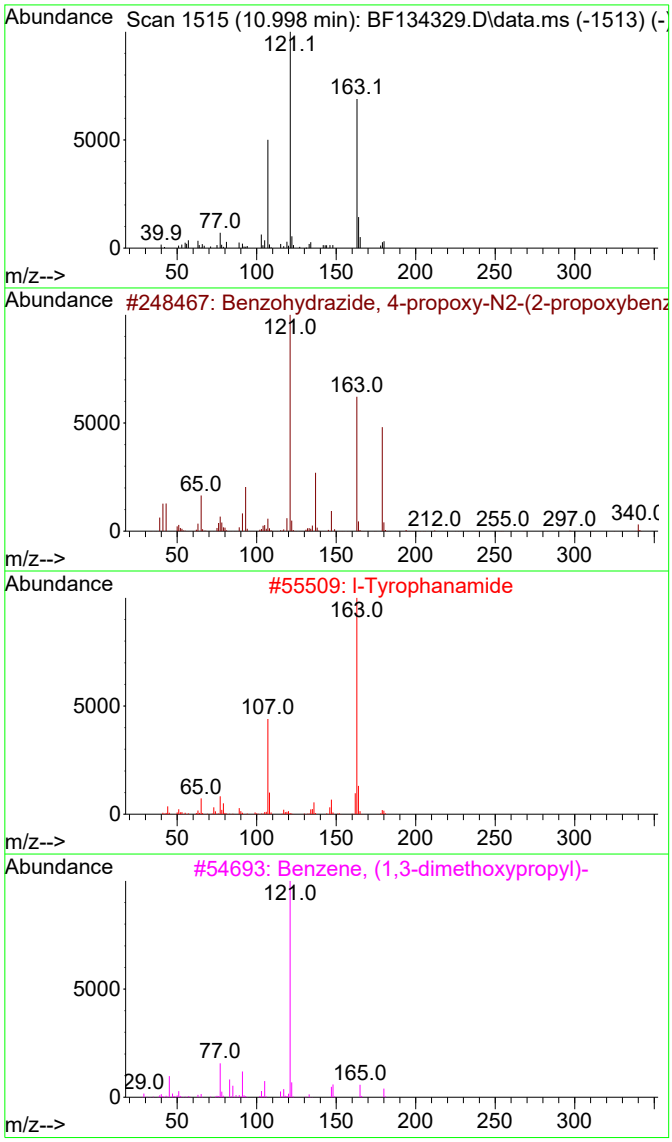
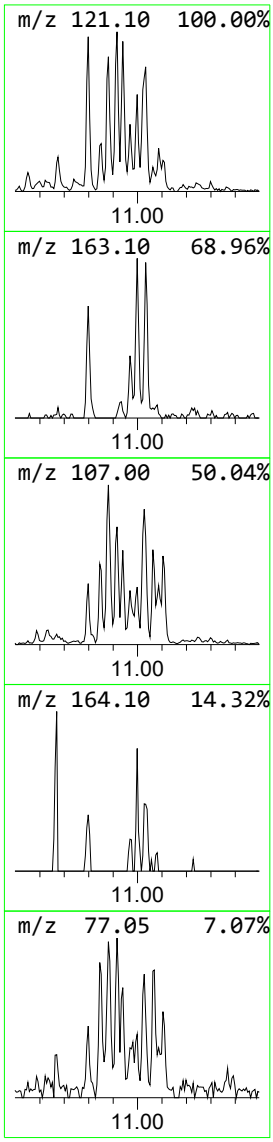
Peak Number 8 unknown10.998 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.998	2.43 ng	58375	Phenanthrene-d10	11.369

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzohydrazide, 4-propoxy-N2-(2-...	340	C20H24N2O3	1000258-67-8	42
2	l-Tyrophanamide	180	C9H12N2O2	1000131-25-3	38
3	Benzene, (1,3-dimethoxypropyl)-	180	C11H16O2	1000327-31-8	35
4	ortho-Hydroxypropiophenone	150	C9H10O2	000610-99-1	25
5	Tricyclo[3.3.1.1(3,7)-]decane, 1...	242	C12H19Br	000941-37-7	23





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BNA_F
ClientSampleId :
RB-42-(1-3)

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TIC Integration Parameters: LSCINT.P

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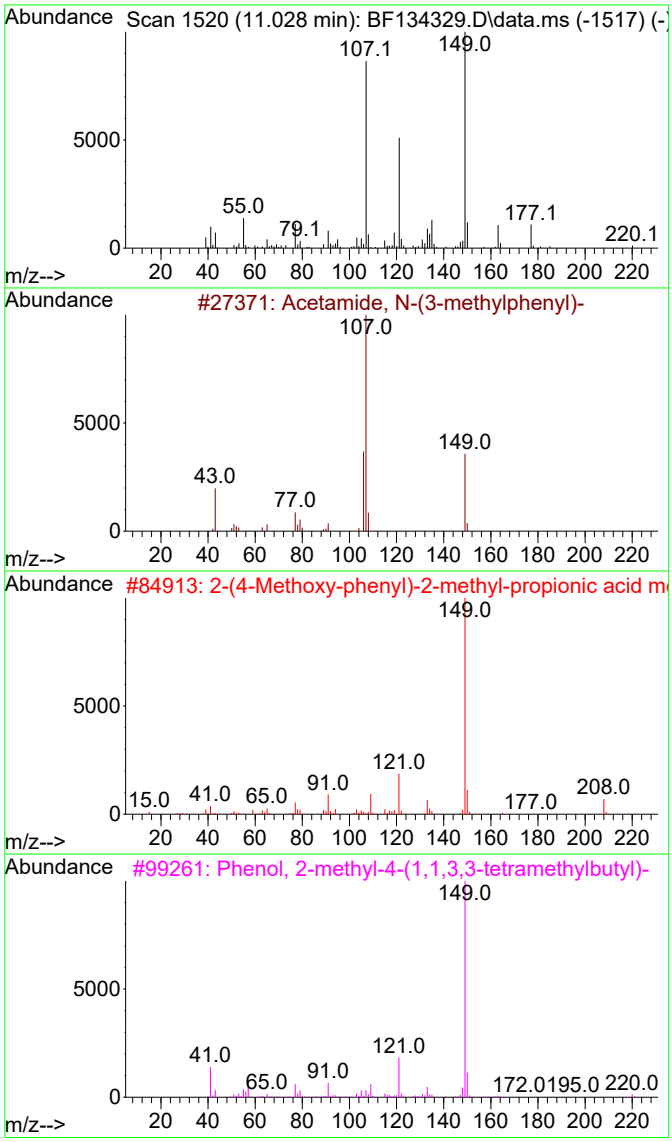
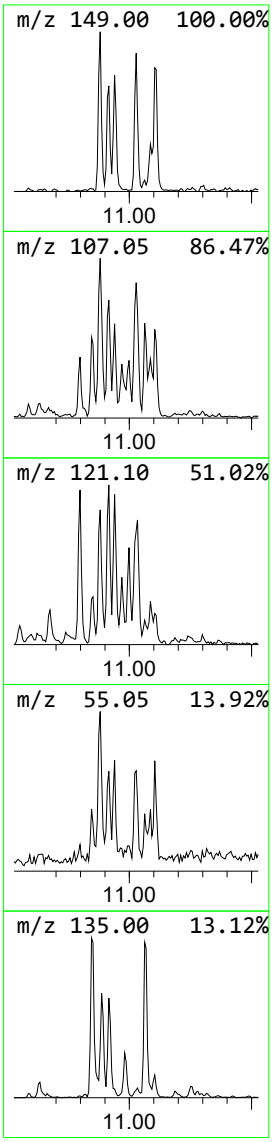
Peak Number 9 Acetamide, N-(3-methylphenyl)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.028	7.32 ng	175761	Phenanthrene-d10	11.369

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetamide, N-(3-methylphenyl)-	149	C9H11NO	000537-92-8	64
2	2-(4-Methoxy-phenyl)-2-methyl-pr...	208	C12H16O3	006274-50-6	38
3	Phenol, 2-methyl-4-(1,1,3,3-tetr...	220	C15H24O	002219-84-3	38
4	1-Methyl-3-ethyladamantane	178	C13H22	001687-34-9	38
5	Methyl (1s,3s,5R,7S)-3-methylada...	208	C13H20O2	1010504-39-1	38





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ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RB-42-(1-3)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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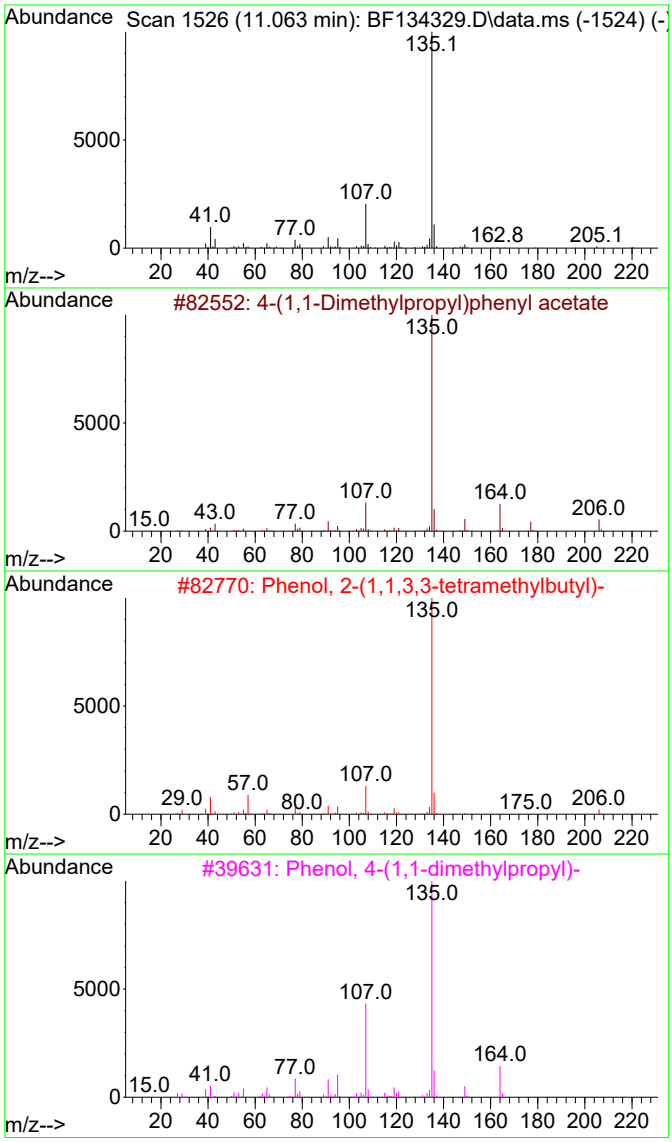
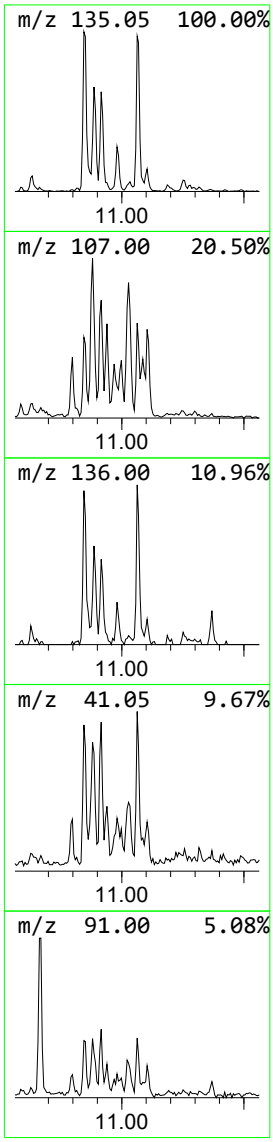
Peak Number 10 4-(1,1-Dimethylpropyl)pheny... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.063	7.69 ng	184667	Phenanthrene-d10	11.369

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-(1,1-Dimethylpropyl)phenyl ace...	206	C13H18O2	1000373-45-3	83
2	Phenol, 2-(1,1,3,3-tetramethylbu...	206	C14H22O	003884-95-5	78
3	Phenol, 4-(1,1-dimethylpropyl)-	164	C11H16O	000080-46-6	78
4	Phenol, 4-(1,1,3,3-tetramethylbu...	206	C14H22O	000140-66-9	72
5	Hexestrol	270	C18H22O2	000084-16-2	72





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Operator : CG\JU
Sample : 03597-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RB-42-(1-3)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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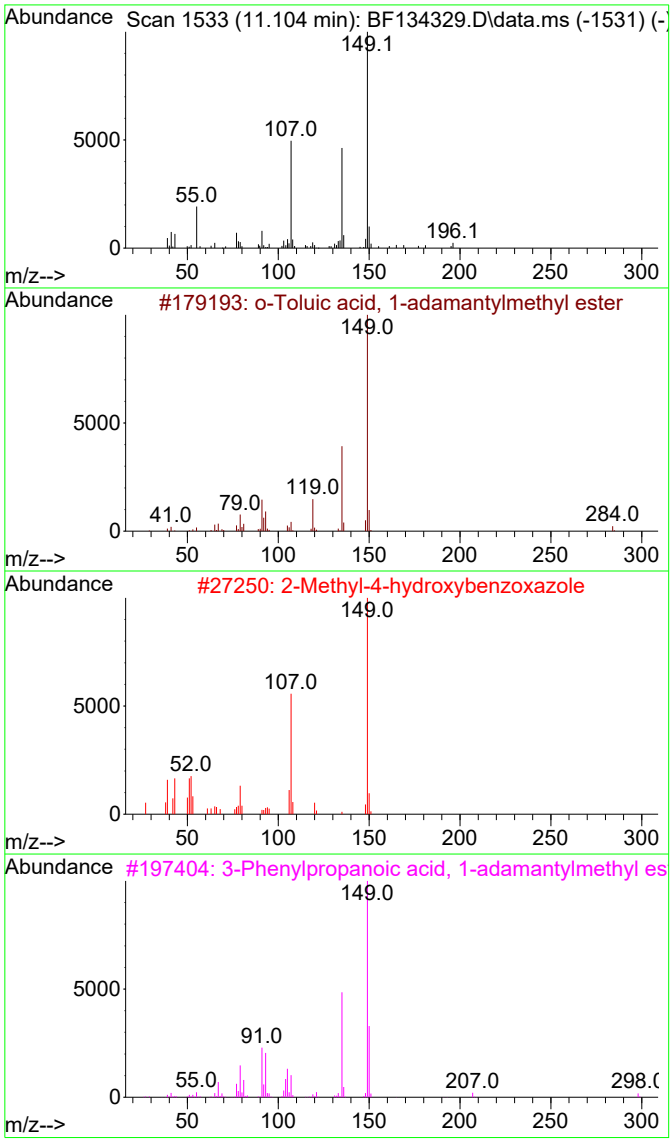
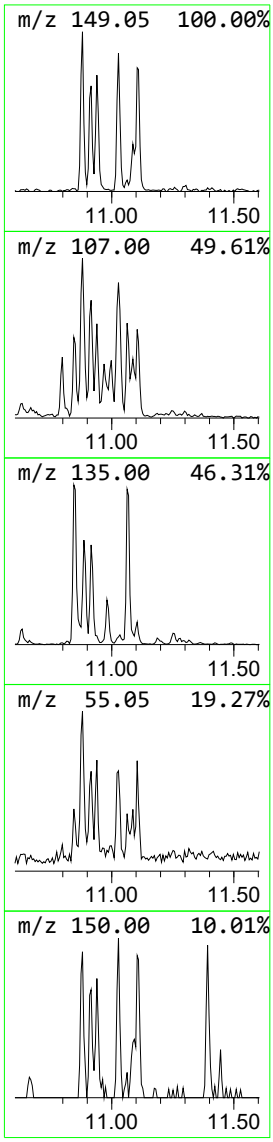
Peak Number 11 o-Toluic acid, 1-adamantylm... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.104	4.03 ng	96795	Phenanthrene-d10	11.369

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	o-Toluic acid, 1-adamantylmethyl...	284	C19H24O2	1000292-22-6	53
2	2-Methyl-4-hydroxybenzoxazole	149	C8H7NO2	051110-60-2	50
3	3-Phenylpropanoic acid, 1-adaman...	298	C20H26O2	1000282-93-6	42
4	Phthalic acid, 2-(2-nitrophenyl)...	427	C24H29NO6	1000377-99-8	35
5	1H-S-Triazolo[1,5-a]pyridin-4-iu...	149	C7H7N3O	013980-64-8	32





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Instrument :
BNA_F
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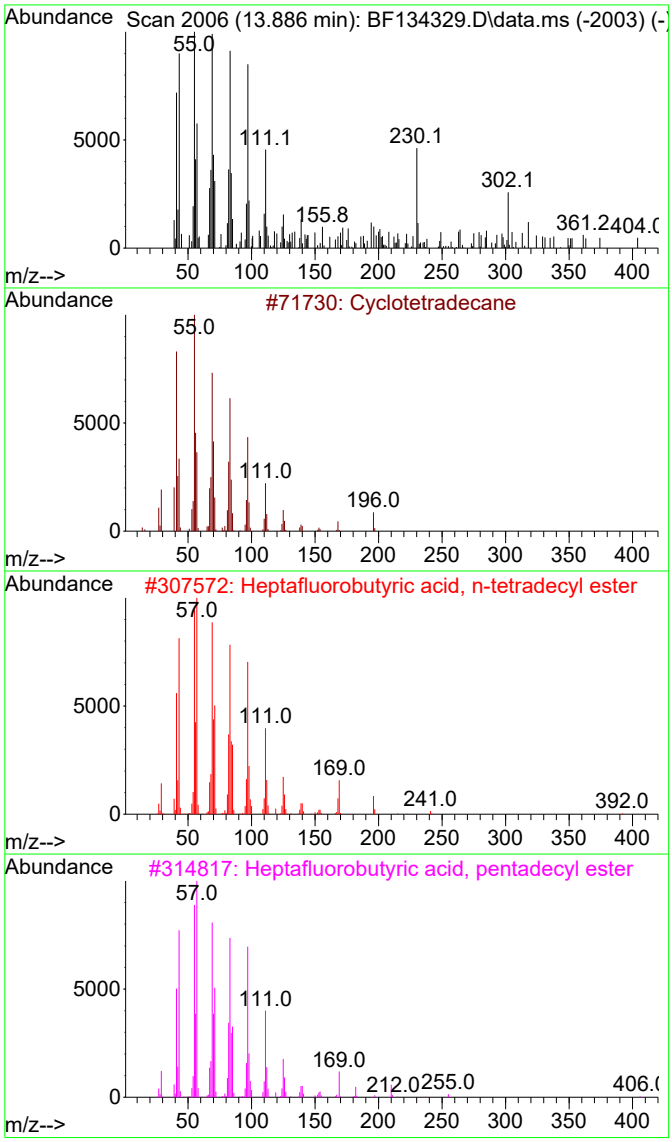
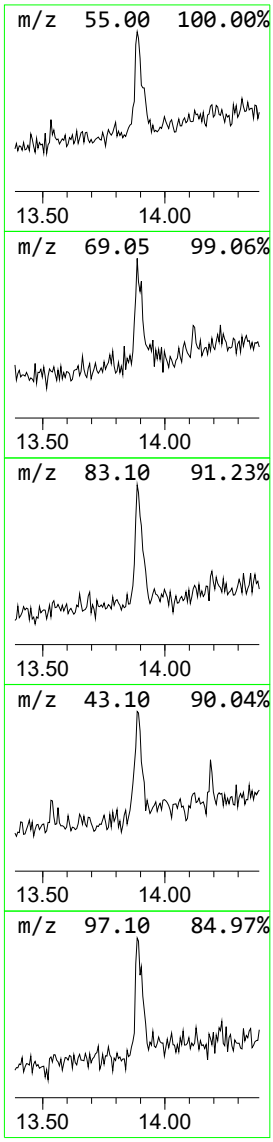
Peak Number 12 Cyclotetradecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.886	4.90 ng	92212	Chrysene-d12	14.027

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclotetradecane	196	C14H28	000295-17-0	90
2	Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	76
3	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	68
4	Pentafluoropropionic acid, tetra...	360	C17H29F5O2	006222-06-6	68
5	5-Tetradecene, (E)-	196	C14H28	041446-66-6	60





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071723\
Data File : BF134329.D
Acq On : 17 Jul 2023 22:38
Operator : CG\JU
Sample : 03597-01
Misc :
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Instrument :
BNA_F
ClientSampleId :
RB-42-(1-3)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Ethanol, 2-(2-e...	6.669	2.0	ng	41877	1	6.840	415601	20.0
1-(Isocyanatome...	10.798	3.2	ng	77324	4	11.369	480257	20.0
Phenol, 4-(1,1,...	10.845	7.8	ng	186625	4	11.369	480257	20.0
unknown10.881	10.881	10.4	ng	249176	4	11.369	480257	20.0
4-(7-Methylocty...	10.916	8.3	ng	200579	4	11.369	480257	20.0
unknown10.939	10.939	4.4	ng	105539	4	11.369	480257	20.0
Butane, 1,3-dib...	10.980	3.7	ng	87797	4	11.369	480257	20.0
unknown10.998	10.998	2.4	ng	58375	4	11.369	480257	20.0
Acetamide, N-(3...	11.028	7.3	ng	175761	4	11.369	480257	20.0
4-(1,1-Dimethyl...	11.063	7.7	ng	184667	4	11.369	480257	20.0
o-Toluic acid, ...	11.104	4.0	ng	96795	4	11.369	480257	20.0
Cyclotetradecane	13.886	4.9	ng	92212	5	14.027	376176	20.0